Physical Chemistry

AN EXPERIMENTAL & THEORETICAL STUDY OF ALKALI CATIONL/METHIONINE INTERACTIONS

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The interaction of alkali metal cations ($M^+ = K^+$, Na^+, Li^+) with the amino acid methionine (MET) is examined in detail. Experimentally, the bond energies are determined using threshold collision-induced dissociation of the M^+(MET) complexes with Xe using a guided ion beam mass spectrometer. Analyses of the energy dependent cross sections provide 0 K bond energies of 3.33 $\pm$ 0.18 eV, 2.09 $\pm$ 0.11 eV, and 1.47 $\pm$ 0.11 eV for the Li^+, Na^+, and K^+ MET complexes, respectively. All bond energy determinations include consideration of unimolecular decay rates, internal energy of reactant ions, and multiple ion-molecule collisions. Ab initio calculations at the MP2(full)/6-311+G(2d,2p), B3LYP/6-311+G(2d,2p), and B3P86/6-11+G(2d,2p) levels (with geometries and zero point energies calculated at the B3LYP/6-311G** level) show good agreement with the experimental bond energies, e.g., the MP2 values (without basis set superposition error corrections) are 3.08 eV, 2.14 eV, and 1.54 eV, respectively. Subtle changes to the MET side chain orientation are found to cause noticeable changes in energy. The combination of this series of experiments and calculations allows for the impact of the functional groups of the methonine on the overall binding strength to be thoroughly explored.